



Simulation of a porous medium (PM) engine using a two-zone combustion model

Hongsheng Liu*, Maozhao Xie, Dan Wu

School of Energy and Power Engineering, Dalian University of Technology, Dalian 116024, China

ARTICLE INFO

Article history:

Received 26 June 2008

Accepted 8 April 2009

Available online 14 April 2009

Keywords:

Porous medium (PM) engine

Two-zone model

Numerical simulation

ABSTRACT

Porous medium (PM) engine was a new type engine based on the technique of combustion in porous medium, which can realize homogeneous and stable combustion. In this paper, the combustion and working processes of a specific PM engine were simulated by a two-zone model considering the influences of the mass distribution, heat transfer from the cylinder wall, mass exchange between zones and the heat transfer in porous medium. Influences of operating parameters, e.g. intake temperature and pressure, compression ratio, the excess air ratio on the performance of the PM engine were discussed. It was found out that the porous medium, acting as a heat recuperator, can significantly enhance the evaporation of liquid fuel and preheat the mixture, which promotes the ignition and combustion in the cylinder; and that the initial PM temperature and the compression ratio are critical factors controlling the compression ignition of the mixture.

© 2009 Elsevier Ltd. All rights reserved.

1. Introduction

Homogeneous charge and compression ignition (HCCI) is one of the most attractive combustion modes for automotive engines to achieve both high efficiency and low NO_x and particulate emissions. Despite many advantageous features of the HCCI combustion, it still fronts some challenges including higher HC and CO emissions and expanding operating range. As no external means are used to ignite the mixture, it is especially difficult to control the combustion processes inside the engine [1]. In this respect, the new concept of the so called porous medium (PM) Engine, based on the regenerative or super-adiabatic combustion in a porous medium, offers new ways in dealing with these problems. Recently, the PM engine has received attention from numerous researchers because of its potential for producing homogeneous mixtures and reducing NO_x and soot emissions [2,3].

With HCCI, the start of combustion is mainly controlled by the chemical kinetics, which depends on the charge composition and the pressure and temperature histories of the reactants during the compression process. Thus a detailed chemistry mechanism is essential for modeling HCCI combustion [4,5]. Various types of models have been developed to simulate HCCI combustion including single-zone, multi-zone and multi-dimensional models.

Single-zone models [6] treat the entire cylinder as a homogeneous reactor with uniform temperature, pressure and compositions. Because single-zone models represent the highest temperature regions in the cylinder, the burn point can be well predicted within different operating ranges. However, the inhomogeneity of temperature and compositions within the cylinder are not taken into account, so peak pressure, burn duration and the amount of emissions could not be accurately predicted. Multi-zone models [7,8] divide the cylinder into a number of zones with different temperatures and compositions. With the interaction between zones and detailed chemical kinetics mechanism being considered, the combustion process is reproduced. Multi-zone models can, with moderate computation costs, provide results in better agreement with experiments than single-zone models due to consider temperature and compositions inhomogeneity in the cylinder. Because of these advantages the multi-zone models have found wide applications in the engineering. Multi-dimensional models [9,10] combine detailed chemical kinetics and engine computational fluid dynamics (CFD) to simulate HCCI combustion. However, a coupled CFD and detailed chemistry simulation requires substantial memory and CPU time which might be impractical for current computer capabilities.

Development of porous burners has been encouraged by lower emission standards in recent years. As a burner of liquid fuel, porous medium is also an efficient evaporator. Combination of large heat capacity of the porous material, large specific surface area with excellent heat transfer in PM volume makes the fuel droplets vaporization very fast and complete. The collision of the fuel droplets within the complex porous structure contributes to very effective mixture formation and homogenization, which ensures a homogeneous combustion in the PM volume. Liquid vaporizing combustion in porous medium burner has fine flame stability and characteristic of low emission, which has been proved by experimental and numerical research [11–13]. Sumrerng and Narongsak [11] built a simple porous burner system for burning kerosene. The evaporation mechanism and the combustion

* Corresponding author. Tel.: +86 411 8470 6302; fax: +86 411 8470 8460.

E-mail address: lhsh@dlut.edu.cn (H. Liu).

characteristics occurring in the burner were studied by measuring thermal structures in terms of temperature profiles along the centerline of the porous burner. Echigo and Martynenco [12] studied the phenomenon of self-sustaining combustion of a gaseous mixture in inert highly porous medium with prior vaporization of liquid droplets numerically. Combustion and several heat transfer modes as well as droplet behavior in porous medium were investigated combinedly. Kayal and Chakravarthy [13] developed a one-dimensional heat transfer model to analyze the combustion of liquid fuel (kerosene) inside an inert porous medium under steady state conditions using a single step global reaction mechanism.

Based on these previous researches, a new concept of controllable combustion in porous media for internal combustion engine has been suggested and developed [14–16]. Hanamura et al., [14] designed a reciprocating heat engine, similar to a Stirling engines, based on the technique of super-adiabatic combustion in porous media. One-dimensional numerical simulations showed that the thermal efficiency of the engine reached to 57.5% with a compression ratio between two and three, which is much lower than those of conventional Otto and diesel cycles. Weclas [15] suggested a strategy for development of intelligent combustion systems for IC engines, whose essence involved a new concept for mixture formation and homogeneous combustion based on the PM combustion technology. Durst [16] proposed two structural versions for PM engine design. In order to prove the feasibility of the PM engine, they modified a single-cylinder, air cooled diesel engine to incorporate a PM in the cylinder head and operated it as a PM engine. The engine was operated for several hours without any damage to the PM material or showing any uncontrolled operations. The experiments showed very low emission level for the test engine and much lower combustion noise due to the reduction in the pressure peak compared to conventional DI engines. However, no data for performance of PM engines are available in the open literature.

Referring to the design of Durst [16], this paper presents a two-zone model to investigate the combustion process of the PM engine. A computer program was developed and coupled with the chemical kinetics package CHEMKIN III. In this way a skeletal kinetic mechanism for iso-octane oxidation including 38 species and 69 elementary reactions was used for the chemistry simulation, which could predict satisfactorily ignition timing, burn rate and the emissions of HC, CO and NO_x for HCCI engine [17].

2. Mathematical model

2.1. Working principle of PM engine

The PM engine is here defined as an internal combustion engine with a highly porous medium (PM) chamber mounted on the cylinder head (Fig. 1). Same components as in conventional internal combustion engines are still used in the PM engine, except the fuel injection system that is required to be modified and optimized.

In the “permanent contact” PM engine the PM chamber always contacts with the cylinder and its operation is the same with a traditional diesel engine. In the “period contact” PM engine, the PM chamber is equipped with a valve permitting a periodic contact between the PM chamber and the combustion chamber. At the end of expansion stroke the valve is closed and fuel is injected into the PM volume, the process continues through exhaust, intake and compression strokes. The large specific surface area of the PM and excellent heat transfer in the PM volume as well as a long time available for fuel vaporization make the liquid fuel vaporized completely. At the end of compression (near the TDC), the valve of the PM chamber opens and the compressed air flows from the cylinder into the hot PM volume containing fuel vapors, generating a highly turbulent flow condition. Very fast fuel–air mixing occurs and the resulting mixture is self-ignited across the whole PM volume. The

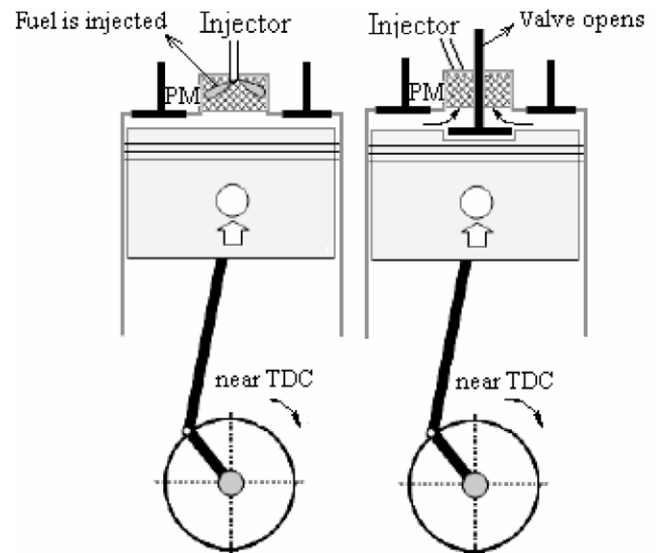


Fig. 1. Principle of the PM-engine cycle. (Left) permanent contact PM engine, and (Right) period contact PM engine.

heat released from the combustion process is partly deposited in the PM volume, which could be used to vaporize fuel and preheat the mixture in the next cycle. The cylinder and the PM chamber keep separated during the intake, compression and exhaust strokes, which make this type of PM engines operate as a conventional DI engine in these strokes.

The main difference between the two type PM engines is whether the compressed air contacts with fuel vapors during its evaporation, which decides the ignition timing.

The formation of homogeneous mixture and 3D-thermal self-ignition in the PM volume create a realizable condition for homogeneous combustion, which is almost independent of the engine load. Furthermore, the heat recuperation in the PM may be used for heating up the compressed air and controlling the combustion temperature level.

2.2. Computational model

In the present model the combustion chamber is divided into two zones (Fig. 2) with different temperatures and mass compositions according to the structure of the PM engine: the PM chamber zone (zone one) and cylinder zone (zone two). During the combustion process the volume of PM zone keeps constant while the volume of cylinder zone varies with time (crank angle). The thermodynamic properties and mass composition are spatially

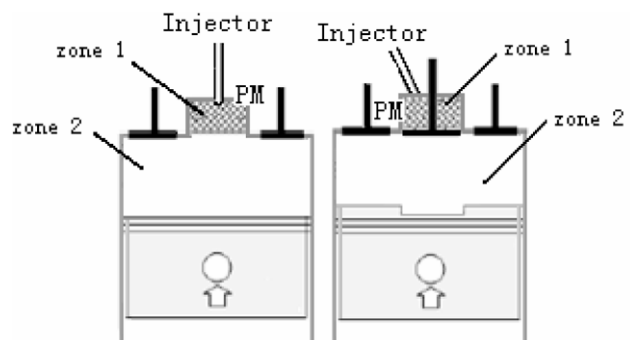


Fig. 2. The definition of two zones in different engine. (Left) in permanent contact PM engine, and (Right) in period contact PM engine.

uniform in each zone. Moreover, mass exchanged between two zones occurs to maintain the in-cylinder pressure uniform.

For simplicity, the following assumptions are introduced in the formulation:

(a) The porous medium with high porosity is homogeneous, continued and non-catalytic [11,13].

For the period contact PM engine: (b) Fuel droplets have vaporized completely before the valve is open due to the excellent heat properties of PM volume and the long time available for fuel vaporization [15,16]. Consequently the temperature of air, fuel vapor and the solid in the PM chamber are uniform as the valve is open. (c) When the valve is open, the highly compressed air is assumed to be mixed with the fuel vapor immediately to form a homogeneous combustible mixture because the pressure in cylinder chamber is much higher than that in the PM chamber.

For permanent contact PM engine: (d) All fuel droplets have the same diameter and are uniformly distributed within the PM volume when fuel is injected in the PM chamber. Through the vaporization process the total number of fuel droplets decreases while the diameter keeps constant, which influences the mass fraction of fuel vapor [12]. (e) The heat transfer between the PM solid and droplets is negligible for little probability of contact between each other.

2.2.1. Thermodynamics and chemical kinetics model

In the thermodynamic model the mass of each zone is assumed to be constant and species are assumed to obey the ideal gas equation of state. According to the first law of thermodynamics (FLT), the energy equations of each zone can be written as:

$$\dot{Q}_i = m_i \bar{c}_{v,i} \frac{dT_i}{dt} + p_{cyl} \frac{dV_i}{dt} \quad (1)$$

The in-cylinder pressure at each time step is calculated using the ideal gas relation [8] for all the zones:

$$p_{cyl} = \left(\sum_{i=1}^2 m_i \bar{R}_i T_i \right) / (V_{cyl} + \varepsilon V_{PMB}) \quad (2)$$

Substituting Eq. (2) into (1) yields:

$$\frac{dT_i}{dt} = \frac{1}{\bar{c}_{v,i}} \left[\dot{q}_{chem,i} + \dot{q}_{loss,i} + \dot{q}_{PM,i} - \frac{\sum_{i=1}^2 m_i \bar{R}_i T_i}{m_i (V_{cyl} + V_{PMB})} \cdot \frac{dV_i}{dt} \right] \quad (3)$$

In Eqs. (1)–(3), m_i , T_i , V_i , $\bar{c}_{v,i}$, $\bar{R}_i$ and $\dot{Q}_i$ are mass, temperature, volume, specific heat capacity at constant pressure, universal gas constant and heat release in each zone i , respectively. V_{PMB} is volume of the PM chamber, and ε is the porosity of the PM. The cylinder volume V_{cyl} and its variation rate dV_{cyl}/dt can be described by functions of crank angle and cylinder size [18]. For unit mass of the mixture in the single zone i : $\dot{q}_{chem,i}$ is heat release of chemical reaction, $\dot{q}_{loss,i}$ is heat loss through the cylinder wall into the surroundings, $\dot{q}_{PM,i}$ is the total heat transfer in the PM between gas and liquid as well as gas and solid, where $dV_i/dt = 0$ for $i = 1$, $dV_i/dt = dV_{cyl}/dt$ and $\dot{q}_{PM,i} = 0$ for $i = 2$.

The chemical heat release in each zone is obtained by the following method.

For each species j in zone i , a set of differential equations for species mass fraction $Y_{j,i}$ is solved using the CHEMKIN III libraries to obtain the change in mixture composition [8,9]:

$$\frac{dY_{j,i}}{dt} = \dot{\omega}_{j,i} v_i W_{j,i} + \delta_{ij} \cdot \dot{m}_f v_i \quad (4)$$

where $\dot{\omega}_{j,i}$ is the molar rate of production calculated by CHEMKIN [19]. v_i is the average specific volume of zone i . $W_{j,i}$ is molecular weight of species j in zone i .

For the permanent contact PM engine, the evaporation and chemical reaction take place in PM zone at the same time. The mass fraction of fuel vapor is controlled by both chemical kinetics and evaporation rate of fuel droplets in PM chamber. Thus, when $i = 1$ and $j = ifuel$ a coefficient $\delta_{ij} = 1$ is enrolled where $ifuel$ represents the species of fuel, and $\delta_{ij} = 0$ otherwise. $\dot{m}_f$ is the evaporation rate of fuel droplets, and is given in model of evaporation.

For the period contact PM engine $\delta_{ij} = 0$, because the evaporation is separated from the chemical reactions and has been finished before the valve is open.

The chemical heat release of zone i is obtained as:

$$\dot{q}_{chem,i} = \sum_{j=1}^K u_{j,i} \frac{dY_{j,i}}{dt} = \sum_{j=1}^K u_{j,i} (\dot{\omega}_{j,i} v_i W_{j,i} + \delta_{ij} \cdot \dot{m}_f v_i) \quad (5)$$

where $u_{j,i}$ is specific internal energy of species j in zone i . δ_{ij} has the same value as in Eq. (4).

The overall wall heat loss $\dot{q}_{loss,i}$ can be determined by a heat transfer model for the HCCI engine, especially. The heat transfer in the PM $\dot{q}_{PM,i}$ can be obtained similarly by a heat transfer model for the PM.

Eq. (3) provides two equations for the two zones. The variation of the mean temperature in each zone dT_i/dt can then be calculated when parameters m_i , $\bar{R}_i$, T_i , $\bar{c}_{p,i}$, $\dot{q}_{chem,i}$, $\dot{q}_{PM,i}$, $\dot{q}_{loss,i}$ for the gas mixture and V_{cyl} , dV_{cyl}/dt for the engine are given. Combining with the species mass fraction (Eq. (4)) for each zone, an equation set of $2(K+1)$ order is built. Giving the initial conditions, variations in temperatures and species mass fractions can be obtained by solving the equation set with the DVODE package from CHEMKIN which is a variable-coefficient Ordinary Differential Equation solver, with fixed-leading coefficient implementation.

In the above calculation, the mass transferred between zones is not considered. Thus, a special model is needed for computing the mass exchange at the end of each time step to redistribute the mass of each zone and keep the in-cylinder pressure uniform.

For HCCI engines, it was found that the time step of 0.5 CAD is small enough [9]. In the following calculations, the time step is taken to be 0.4 CAD before ignition and 0.06 CAD during the combustion process, which is adequate for predicting the temperature distribution and evolution.

2.2.2. Heat transfer model for cylinder wall

It is well known that modeling of wall heat losses in HCCI combustion processes is a very challenging task. The overall wall heat loss is defined as:

$$\frac{dQ_w}{dt} = -hA(T - T_w) \quad (6)$$

where h , A and T_w are heat rate coefficient, combustion chamber area and wall temperature, respectively.

According to the experimental results reported for the gasoline HCCI process, the improved Woschni model of Chang [20] showed very good performance for the prediction of heat transfer in HCCI engine. The heat transfer rate coefficient is written as:

$$h = 129.8B^{-0.2}p^{0.8}T^{-0.73}\omega^{0.8} \quad \text{with :}$$

$$\omega = C_1 \bar{v} + \frac{C_2}{6} \frac{V_d T_r}{P_r V_r} (P - P_{mot})$$

where B is the cylinder bore, T is mean gas temperature, C_1 and C_2 are constants in the Woschni heat transfer model and ω is mean gas velocity defined as function of average velocity of piston $\bar{v}$, cylinder volume V_d , referenced temperature T_r , pressure p_r , volume V_r , and motoring pressure p_{mot} .

2.2.3. Modeling of fuel evaporation

2.2.3.1. For permanent contact PM engine. Since modern nozzles are able to produce a fuel spray with a mean diameter in the order of

10 μm , the initial diameter 100 μm is considered in this study. Therefore, the average size of the fuel droplets is small enough compared to the average pore size of the PM. As assumed, the contact heat transfer between liquid and solid is neglected. Furthermore, the radiative heat transfer of the solid to the droplets is not taken into account as the temperature of gas is higher than that of the solid during the fuel injection. The heat transfer between gas and solid is dominant, the heat transfer between gas and liquid are also considered.

When the temperature of liquid is lower than its saturation temperature, the energy equation for liquid phase [12] is written as:

$$\varepsilon \rho_f c_l \frac{dT_l}{dt} = \gamma_{gl}(T_g - T_l) \quad (7)$$

where γ_{gl} is the volumetric heat transfer coefficient between gas and liquid. T_l is the temperature of liquid droplet. $\rho_f = \rho_l n (\pi d^3/6)$ is the density of fuel. d and n is the mean diameter and the number density of liquid droplets, respectively. ρ_l is the material density of liquid.

The volumetric heat transfer coefficient between gas and liquid per unit volume is defined as $\gamma_{gl} = n \cdot \varepsilon \cdot h_{gl} \cdot S_d$ [12], where h_{gl} is convective heat transfer coefficient between liquid and gas and S_d is the specific surface of a liquid droplet. The number density of liquid droplet n is given as: $n = \frac{m_{liquid}}{\rho_l \cdot (\pi d^3/6) \cdot \varepsilon \cdot V_{PMB}}$, where m_{liquid} is the mass of liquid fuel contained in the space of porous medium. The initial value of n is determined by the total mass of fuel injected per cycle and a given droplet diameter. With the progress of evaporation, n decreases until to zero. Because inside the PM turbulence has only a weak effect, assuming the Nusselt number [12] $Nu_{gl} = h_{gl} d / \bar{\lambda}_g = 2$, and h_{gl} can be calculated. Thus, the volumetric heat transfer coefficient between gas and liquid can be described as:

$$\gamma_{gl} = \frac{1}{4} n \pi d Nu_{gl} \cdot \bar{\lambda}_g \quad (8)$$

The evaporation rate of fuel droplets $\dot{m}_f$ is given as:

$$\dot{m}_f = \gamma_{gl}(T_g - T_{sat})/L \quad (9)$$

where γ_{gl} is the volumetric heat transfer coefficient between gas and liquid, T_g is the temperature of gas mixture, T_{sat} is the saturation temperature of solvent–fuel mixture and L is the latent heat of evaporation.

2.2.3.2. For period contact PM engine. For the period contact PM engine, the evaporation process of liquid fuel occurs in PM chamber during the valve keeps closed. Thus, the evaporation process is decoupled from the cylinder, and it is not necessary to study the detailed evaporation process. The most important problem is then the thermodynamic properties of gas mixture and solid matrix at the time of the valve opening. Here, it is assumed that the temperature of porous solid and fuel vapor at the valve opening are uniform because a long time available for evaporation and heat transfer within the PM. The temperature inside a fuel droplet is also assumed uniform, but varies with time. The stress of the evaporation process is put on calculation of the heat transfer between gas–solid and gas–liquid in PM chamber since the valve was closed, whereas the evaporation rate of liquid droplets is not mentioned here. The heat balance equation for the closed PM chamber can be formulated as follows:

$$\rho_s c_s (T_{sc} - T_{open}) + \rho \varepsilon c (T_{gc} - T_{open}) = m_f c_l (T_{sat} - T_l) + m_f L + c_{evap} m_f (T_{open} - T_{sat}) \quad (10)$$

where ρ_s and ρ are the densities of the PM and remained gas in the PM chamber, respectively. T_{sc} and T_{gc} are the temperatures of the

solid and gas in the PM chamber when the valve closed at former cycle. T_{open} is the temperature of vapor and solid in PM chamber as the valve was open, which can be calculated by Eq. (10). m_f is the total mass of fuel injected per cycle, which is determined by the mass of intake air and a specific equivalence ratio. c_s , c , c_l and c_{evap} is the specific heat of solid, remained gas, fuel droplet and fuel vapor in the PM chamber, respectively.

2.2.4. Heat transfer modeling in porous medium

2.2.4.1. For permanent contact PM engine. For the permanent contact PM engine, the heat transfer associated with liquid droplet during evaporation should be considered in the model of heat transfer in porous medium.

The total heat transfer in porous medium $\dot{q}_{PM,i}$ can be described with the following equation:

$$\dot{q}_{PM,i} = [\gamma_{gs} \cdot (T_s - T_g) - (1 - \delta) \gamma_{gl}(T_g - T_l) - \delta \cdot \dot{m}_f \cdot L - \delta \cdot c_{evap} \cdot \dot{m}_f \cdot (T_g - T_{sat})] / \rho \quad (11)$$

where T_g and T_s are the temperatures of gas mixture in the porous space and the solid porous media, respectively. γ_{gs} is the volumetric heat transfer coefficient between solid and gas. c_{evap} is specific heat of fuel vapor and ρ is the density of gas mixture in porous space. δ is a coefficient of evaporation, $\delta = 0$ for $T_l < T_{sat}$ and $\delta = 1$ for $T_l = T_{sat}$ [12].

Energy equation for solid phase [21] is:

$$\rho_s c_s \frac{dT_s}{dt} = \gamma_{gs}(T_g - T_s) \quad (12)$$

In order to get γ_{gs} , a volumetric Nusselt number Nu_v is defined as [12]:

$$Nu_v = \gamma_{gs} D^2 / \bar{\lambda}_g \quad (13)$$

where D is the average diameter of pore, $\bar{\lambda}_g$ is the thermal conductivity of gas mixture. The correlation for the volumetric Nusselt number Nu_v [21] is given by the following correlation: $Nu_v = C Re^m$. Values of $C = 0.187$ and $m = 1.1$ are used, which depend on the pore diameter. For diesel engine, the Reynolds number (Re) is calculated by $Re = B \bar{v} / \bar{\nu}_g$, where $\bar{v}$ is the mean piston speed as the characteristic velocity. B is cylinder bore as the characteristic length, $\bar{\nu}_g$ is the mean kinematic viscosity of gas mixture.

2.2.4.2. For period contact PM engine. For the period contact PM engine, the volume of porous medium keeps in contact with the cylinder as the valve to the PM chamber keeps open. In this study a model for heat transfer in the PM has been developed, which includes an additional energy equations for the solid matrix and calculation of heat transfer coefficient between gas and solid matrix. Because the liquid fuel has been vaporized completely at the valve opening, the heat transfer relate to the liquid phase is neglected. The energy equation for solid phase is the same as in the case of the period contact PM engine.

The heat transferred $\dot{q}_{PM,i}$ to unit mass of the mixture in the PM chamber zone can be expressed as:

$$\dot{q}_{PM,i} = \gamma_{gs} \cdot (T_s - T_g) / \rho \quad (14)$$

2.2.5. Model for mass exchange between two zones

For the both type of PM engines a model for mass transfer between two zones is needed when the PM chamber is coupled with the cylinder. In the present paper, the mass exchange model is adopted and simplified from the model of Komninos and Hountalas [8] based on the assumption of uniform pressure throughout both zones.

At each time step, since the pressure is uniform throughout the cylinder, the pressure at each time step is calculated using the ideal gas relation for zone i:

$$p_{cyl} = m_i \bar{R}_i T_i / V_i, \quad i = 1, 2 \quad (15)$$

Solving Eq. (15) for the mass of each zone and summing for all the zones:

$$m_{cyl} = \sum_{i=1}^2 m_i = p_{cyl} \sum_{i=1}^2 \frac{V_i}{\bar{R}_i T_i} \quad (16)$$

Solving Eq. (16) for the uniform cylinder pressure:

$$p_{cyl} = \frac{\sum_{i=1}^2 m_i}{\sum_{i=1}^2 \frac{V_i}{\bar{R}_i T_i}} \quad (17)$$

where the temperature of each zone T_i is calculated by Eq. (3), V_i , m_i and $\bar{R}_i$ are volume, mass and universal gas constant of each zone.

At each time step the mass of each zone is calculated using the equation of state for ideal gas:

$$m_i = \frac{p_{cyl} V_i}{\bar{R}_i T_i}, \quad i = 1, 2 \quad (18)$$

The mass change of each zone during the time step is therefore:

$$\Delta m_i = m_i - m_i^{previousCA}, \quad i = 1, 2 \quad (19)$$

Calculations in each time step are divided into two parts. First, the change of composition of each zone is computed using thermodynamics and chemical kinetics with the assumption of no mass transfer between two zones. Next, at the end of the step, the sub-routine of mass exchange is called to compute the mass changes to keep the pressure uniform throughout the cylinder, and then renew associated parameters. Therefore, the change of composition of each zone is the result of combustion and mass transfer from another zone.

The mass flowing from one zone to another has the temperature and chemical species composition of the zone from which it originates. Therefore, the exchange of mass will result the transfer of species and enthalpy between different zones.

2.3. Modeling of chemical kinetics

Combustion is described using a skeletal chemical kinetics mechanism for iso-octane oxidation consisting of 38 species and 69 reactions [17]. For each species, the rate of production is calculated and the differential equations of species mass fraction are solved using the chemical kinetics package CHEMKIN III to obtain the changes in mixture composition in each zone. Comparisons with various experimental data, including shock tube, rapid compression machine, jet stirred reactor and HCCI engine, have indicated very good performance of this mechanism over wide ranges of temperature, pressure and equivalence ratio, especially at high pressure and lean equivalence ratio conditions. Application of the skeletal mechanism to a single-zone model of HCCI engine, yielded results substantially identical with those from the detailed mechanism developed by Jia and Xie [17], and furthermore, the computing time was reduced greatly.

2.4. Engine specifications and operating conditions

Following the study by Durst [16], the PM engine simulated in this paper is based on a Cummins B-series engine, which is a typical medium-duty diesel engine. Dec and co-worker [7,22] have conducted systematical experimental investigation on the engine, which was converted for operation in the HCCI mode. The detailed Specifications of the engine is showed in Table 1. Following the suggestion of Sjöberg and Dec [7,22], an effective compression ratio of 16.8 is used for the calculation. For PM engine, the existence of the PM chamber enlarges the total space volume of combustion chamber. Sequentially, the mass of intake air for the PM engine is

Table 1
Engine specifications.

Displacement(single-cylinder)	0.981 l
Bore	102 mm
Stroke	120 mm
Connecting rod length	192 mm
Nominal geometric compression ratio	18:1
Fuel	Iso-octane
Cylinder wall temperature	384.09 K

0 CA is taken to be TDC intake, so TDC combustion is 360°.

larger and the actual compression ratio is smaller than those of the original engine if other parameters keep unchanged.

The baseline operation condition is specified according to the original engine: the intake pressure is maintained at 100 kPa throughout the study, simulating naturally aspirated operation; the intake temperature of air is 320 K, much lower than that in HCCI (400 K) [7,8]; an engine speed of 1200 rpm is used for all operations; the excess air ratio is 1.6; the injection occurs at 352 crank angle for the permanent contact PM engine. Parameters relevant to the PM chamber for both types PM engine are: the initial temperature of the PM volume is 1100 K, which is approximately the average in-cylinder temperature of a common diesel engine; The cylindrical PM chamber mounted on the cylinder head is 40 mm in diameter and 50 mm high; the material of porous ceramic foams is silicon carbide with a porosity of $\varepsilon = 0.87$, density of $\rho_{PM} = 510 \text{ kg/m}^3$, porous diameter of $D = 1.52 \text{ mm}$ and specific heat of $C_{PM} = 824.7 \text{ J/kg K}$ [21]. For the convenience of comparison, all the operating parameters can change separately in the calculation.

3. Results and discussion

It is known that the auto-ignition temperature of hydrocarbon fuels used in engines has often been determined according to the sudden increase in the in-cylinder (including both zones) gas pressure or temperature [7]. As key parameters for controlling the auto-ignition process the change in the in-cylinder gas pressure or temperature are investigated with emphasis in this paper.

3.1. Influence of the initial temperature

Fig. 3 shows effect of the intake temperature on the in-cylinder temperature and pressure in permanent contact PM engine. It can be seen that the crank angle of the auto-ignition in the cylinder zone (zone two) varies significantly with the initial temperature. However, the process of combustion in the PM zone (zone one) shows almost no change with the change in the initial temperature. That is because the hot PM preheats the gas in PM zone, the temperature of gas mixture in the PM zone before combustion is mainly affected by the temperature of PM, which is relatively steady for each cycle.

If the initial temperature is below a certain threshold, the auto-ignition can occur only so late or even not occur that a sharp rise in the pressure curves cannot be observed. The simulation has shown that the minimum initial temperature required for an auto-ignited combustion in the cylinder zone with the present engine configuration and operating conditions should be above 300 K. With increasing the initial temperature, an obvious two-stage ignition process including both low and high temperature kinetics is displayed in Fig. 3. Due to the combustion in the PM zone, the temperature of mixture in the PM zone increases and mass flows from the PM zone into the cylinder zone as computed in the mass transfer model. Subsequently, the mixture in the cylinder zone is ignited, low temperature reactions occur and follow by high temperature reactions after a long time delay. With the change in temperature,

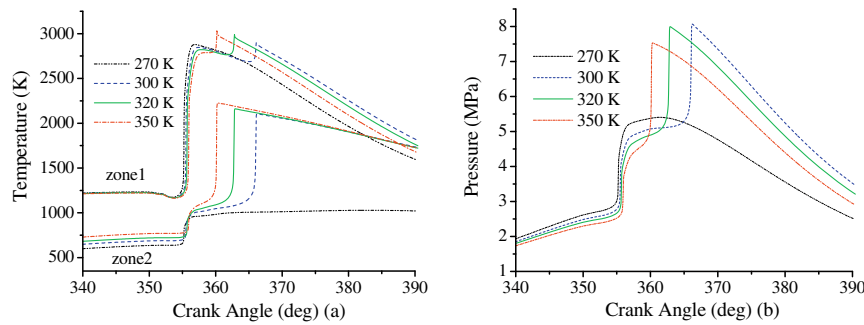


Fig. 3. Effect of the initial temperature on cylinder temperature (a) and pressure (b).

pressure also increases in two stages. The ignition process of the PM engine in the cylinder zone is similar to the HCCI engine.

For a HCCI engine, a fully premixed fueling system is necessary to supply a homogeneous combustible mixture and the initial temperature must be high enough to enable an auto-ignition at the end of compression stroke. In contrary, for the PM engine fuel can be just injected directly into the PM chamber with a lower initial temperature (e.g. 320 K) and the evaporation process occurs in the PM volume and is separated from the cylinder. This is an outstanding advantage of the PM engine. The initial temperature of 320 K was used in the following simulations, unless otherwise stated.

3.2. Influence of the compression ratio

Fig. 4 shows effect of the compression ratio on the in-cylinder temperature in permanent contact PM engine. It can be seen that auto-ignition in the cylinder zone could occur if compression ratio is higher than 13. With increasing compression ratio the ignition point moves ahead and the maximum temperature in the cylinder increases. The calculation indicates that the influence of compression ratio on PM engine is not as strong as on the common HCCI

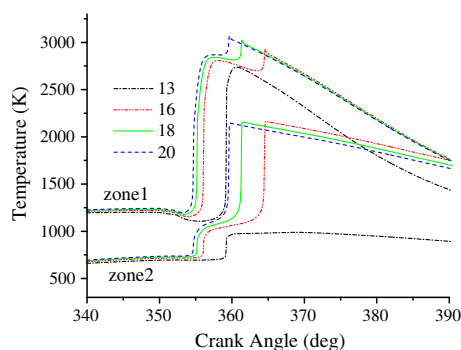


Fig. 4. Influence of the compression ratio on cylinder temperature.

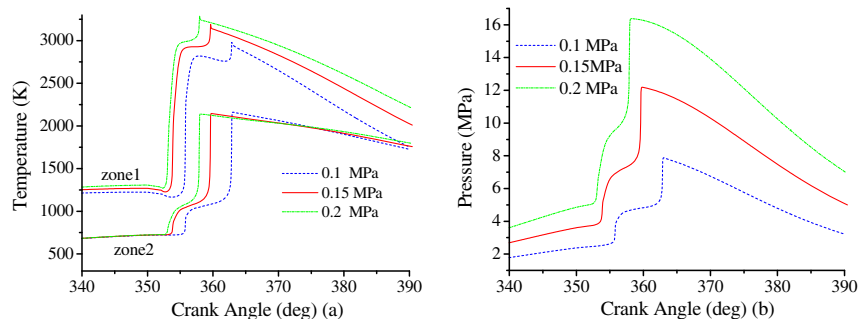


Fig. 5. Influence of the initial pressure on cylinder temperature (a) and pressure (b).

engine. As the combustion starts in the PM zone, mass and heat are transferred from the PM zone to the cylinder zone, which makes ignition and combustion of mixture in the cylinder more easily. In order to attain a reasonable compromise between the power output and emissions of NO_x and HC, it is still important to choose a proper compression ratio to keep the ignition timing nearly at the TDC.

3.3. Influence of the initial pressure

Fig. 5 shows the effect of the initial pressure on the in-cylinder temperature in permanent contact PM engine. For high initial pressure, auto-ignition in the both zones move ahead, especially in the cylinder zone, i.e. the ignition delay between the two zones gets shorter. That is because increasing initial pressure enlarges correspondingly the fuel mass, which results in more combustion heat released in the PM zone and much earlier ignition in the cylinder zone.

In Fig. 5, it is shown that with increasing initial pressure the maximum cylinder pressure increases evidently while the maximum temperature almost shows no change. This means that the thermal efficiency and NO_x emission, being effected greatly by peak temperature, will remain at a relatively steady level when the initial pressure increases. Moreover, the voids in the PM results a lower pressure in the PM engine than that in the HCCI engine, which is beneficial for preventing engine knock. It can therefore be anticipated that boosting intake pressure is an attractive method in the PM engine for higher power output.

3.4. Influence of the excess air ratio

Fig. 6 shows effect of the excess air ratio λ on the in-cylinder temperature and pressure in permanent contact PM engine. For $\lambda = 1.0$, the peak temperature and pressure in the two zones are fairly high and the ignition delay between two zones reaches the minimum. With increasing the excess air ratio, the curves of temperature and pressure trend smooth and the auto-ignition in the

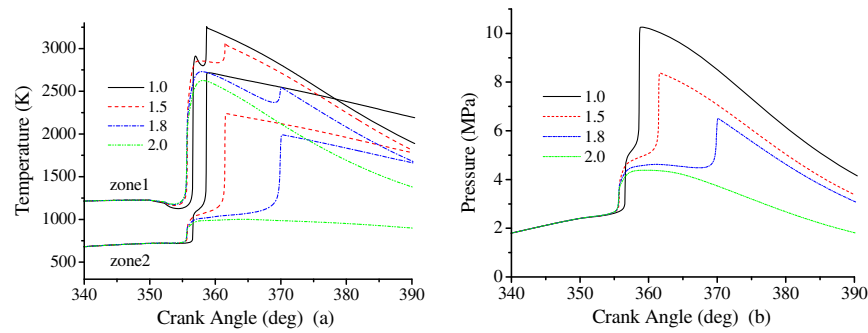


Fig. 6. Effect of the excess air ratio on cylinder temperature (a) and pressure (b).

cylinder occurs very late, until it cannot ignition for $\lambda = 2.0$. Calculation indicates that the combustion efficiency increases with increasing the excess air ratio, because a leaner fuel-air mixture could combust more completely. Furthermore, it is easy to understand that the exhaust concentrations of NO, CO₂ and CO, as functions of the excess air ratio, will also decrease.

In conclusion, a proper excess air ratio must be used to ensure both the occurring of ignition and low emissions for the PM engine.

3.5. Influence of the engine speed

Fig. 7 shows effect of the engine speed on the in-cylinder temperature in permanent contact PM engine. It is showed that the auto-ignition in the PM zone delays about 5 CA and the interval between ignition timings in the two zones gets longer with engine speed increasing from 800 to 2000 rpm. An auto-ignition in the cylinder cannot happen when engine speed reaches 2000 rpm. With increasing engine speed, less time is available for the auto-ignition reactions to take place near the TDC, thus the combustion of mixtures becomes more incompletely. As a result of this, the peak combustion temperature in the PM zone decreases with increased engine speed for the same excess air ratio. It can be noted that for a high speed PM engine one should take some measures in order to realize a complete combustion near TDC, such as boosting pressure or increasing compression ratio.

3.6. Influence of the initial temperature of porous medium

Fig. 8 shows effect of the initial temperature of the porous medium insert on the in-cylinder temperature in permanent contact PM engine. It is clear from Fig. 8 that the PM temperature is a dominating parameter determining the auto-ignition in the PM zone, combustion cannot occur in the PM zone or in the cylinder zone when the initial PM temperature is lower than 900 K. At 1000 K, the combustion occurs in the PM zone, however, ignition in the cylinder zone still could not be realized. Only with farther increase in

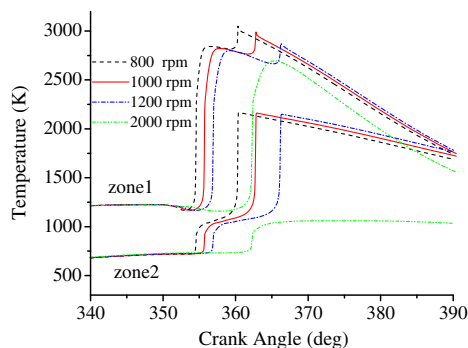


Fig. 7. Effect of the engine speed on cylinder temperature.

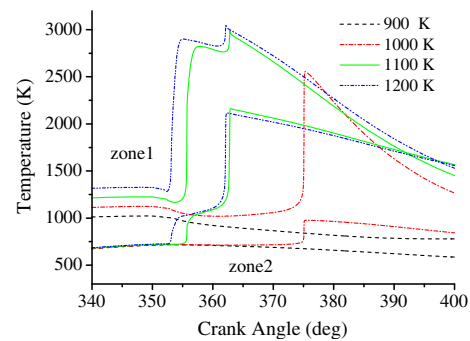


Fig. 8. Effect of the PM temperature on cylinder temperature.

temperature auto-ignition in both zones can succeed. The calculation indicates that the higher the initial PM temperature is, the easier the auto-ignition takes place, at the same time more NO_x emission will be produced. In conclusion, the initial PM temperature is an important factor determining the possibility of ignition, the crank angle of auto-ignition for each zones and the average in-cylinder temperature, which is an important object for PM engine research.

3.7. Mass exchange between zones

Fig. 9 shows variations of the masses contained inside the cylinder zone (zone 2) and PM zone (zone 1) in permanent contact PM engine. The total mass of mixture gas increases during fuel evaporation process, which is shown in detail. In Fig. 9, it is shown that the mass of mixture is mainly distributed in cylinder zone; during compress stroke compressed air flows from the cylinder zone into the PM zone and opposite variety happens during expansion stroke. As combustion occurring in the PM zone near TDC, the temperature and pressure in the PM zone rise sharply and mass flows into the cylinder zone, when the combustion in cylinder happens, mass flows from the cylinder zone to the PM zone. That means that

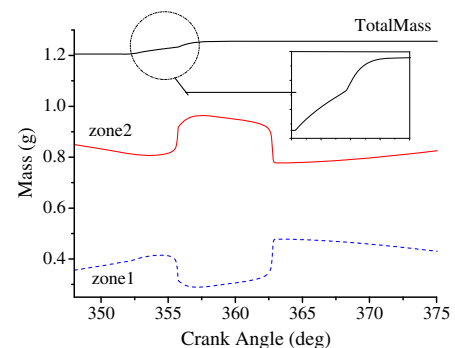


Fig. 9. Mass distributions of two zones.

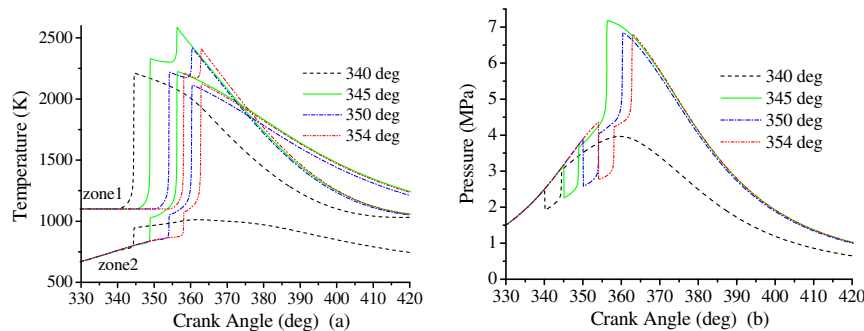


Fig. 10. Effect of the valve opening time on cylinder temperature (a) and pressure (b).

the auto-ignition in both zones is the crucial factor for the mass exchange between two zones. Furthermore, the combustion is controlled by the chemical kinetics model, which means the more fuel mass result the more heat it released, and the calculation also shows that the heat released has same trend with the mass distributing.

3.8. Influence of the valve opening time in the period contact PM engine

For the period contact PM engine, The Influence of the varied parameters (e.g. the compression ratio, engine speed and excess air ratio, etc.) on the temperature of the in-cylinder temperature are approximate to that in permanent contact PM engine, which are not discussed in detail here.

Fig. 10a shows effect of the valve open timing on the in-cylinder temperature in the period contact PM engine. The excess air ratio is 2.0 and the other parameters are same with those in permanent contact PM engine. The maximum temperature is much lower than that in permanent contact PM engine, for a larger excess air ratio is used. It is shown that the combustion in the PM zone follow the valve open and the time delay is about 4 CA. With the increase of valve opening time, the ignition delay between two zones gets shorter.

It is worth to note that, in Fig. 10b there is a sharply drop in pressure when the valve opens. Because the pressure in the PM chamber, which remains its value at the end of former cycle, is much lower than that in the cylinder before the valve opening. The low pressure continues until the combustion in the PM zone happens, and then the pressure increases. The wave of pressure in cylinder might cause shake of the engine, which should be avoided. Moreover, the combustion in cylinder zone has not occurred as the valve open at 340 CA, because the air in cylinder has not got enough compression and its temperature is not high enough to cause auto-ignition.

4. Conclusions

A two-zone model for the new concept internal combustion engine based on the technology of combustion in porous medium is presented in this paper. The main attention is focused on its potential for the realization of a homogeneous combustion process under variable engine operational conditions. The results obtained can be summarized as follows:

1. The PM engine is fueled by direct injection of liquid fuel into the PM chamber with a low initial temperature (300 K) and the evaporation process occurring in the PM volume is separated from the cylinder, for which a premixed fueling system and sufficiently high initial temperature are not need as in the case of HCCI engine.
2. The compression ratio of 13 is great enough for the auto-ignition in the PM zone, which is not so crucial like in the HCCI engine, because the porous medium with high temperature pre-heats the combustible mixture. Besides, the combustion heat released in the PM enhances the ignition in the cylinder. This means that the PM engine could have a wider operation range than a HCCI engine.
3. The auto-ignition timing in the PM zone is dependent mainly on the initial PM temperature, ignition can easily occur as the PM temperature exceeds 1000 K depending on operating conditions. Moreover, the combustion process in the PM zone is relatively steady, which can be controlled by adjusting the initial PM temperature.
4. For the same intake pressure of 1 atm, the pressure in the PM engine is relatively lower than that of a traditional engine due to the voids in PM, boosting in the PM engine may shorten the ignition delay and enlarge the peak pressure with little effects on the peak temperature, which is an attractive method to improve engine output.
5. The average temperature in the PM zone is higher than that in the cylinder, resulting in slightly more emissions of NO for existing excess air ratio of 1.6, which is still a problem for PM engine. In the future research more attention should be paid to lean combustion in the PM engine.

Acknowledgment

This work is supported by the National Basic Research Program of China (Grant Nos. 50736001, 2007CB210002).

References

- [1] X.C. Lu, W. Chen, Z. Huang, A fundamental study on the control of the HCCI combustion and emissions by fuel design concept combined with controllable EGR, *Fuel* 84 (16) (2005) 1074–1092.
- [2] M.Z. Xie, New type of internal combustion engine – super-adiabatic engine based on the porous-medium combustion technique, *Journal of Thermal Science and Technology* 3 (2) (2003) 189–194.
- [3] C.W. Park, M. Kovany, Evaporation–combustion affected by in-cylinder reciprocating porous regenerator, *Transactions of ASME* 124 (2) (2002) 184–194.
- [4] J. Zheng, W. Yang, A skeletal chemical kinetic model for the HCCI combustion process, *SAE Paper* 2002-01-0423, 2002.
- [5] S.M. Aceves, D.L. Flowers, Analysis of premixed charge compression ignition combustion with a sequential fluid mechanics – multizone chemical kinetics model, *SAE Paper* 2005-01-0115, 2005.
- [6] M. Klein, L. Eriksson, A specific heat ratio model for single-zone heat release models, *SAE Paper* 2004-01-1464, 2004.
- [7] M. Sjöberg, J.E. Dec, Potential of thermal stratification and combustion retard for reducing pressure-rise rates in HCCI engines, based on multi-zone modeling and experiments, *SAE Paper* 2005-01-0113, 2005.
- [8] N.P. Komninos, D.T. Hountalas, Description of in-cylinder combustion processes in HCCI engines using a multi-zone model, *SAE Paper* 2005-01-0171, 2005.

- [9] M. Jia, M.Z. Xie, Numerical simulation of HCCI combustion using a multi-dimensional model, *Transactions of CSICE* 25 (1) (2007) 1–8.
- [10] S.C. Kong, R.D. Reitz, Numerical study of premixed HCCI engine combustion and its sensitivity to computational mesh and model uncertainties, *Combustion Theory and Modelling* 7 (2) (2003) 417–433.
- [11] J. Sumrerng, W. Narongsak, The combustion of liquid fuels using a porous medium, *Experimental Thermal and Fluid Science* 26 (6) (2002) 15–23.
- [12] R. Echigo, V.V. Martynenco, Mathematical model of self-sustaining combustion in inert porous medium with phase change under complex heat transfer, *International Journal of Heat and Mass Transfer* 41 (1) (1998) 117–126.
- [13] T.K. Kayal, M. Chakravarty, Modeling of trickle flow liquid fuel combustion in inert porous medium, *International Journal of Heat and Mass Transfer* 49 (11) (2006) 975–983.
- [14] K. Hanamura, K. Bohda, Y. Miyairi, A study of super-adiabatic combustion engine, *Energy Conversion and Management* 38 (3) (1997) 1259–1266.
- [15] M. Weclas, Strategy for intelligent internal combustion engine with homogeneous combustion in cylinder, *Sonderdruck Schriftenreihe der Georg SimonOhm Fachhochschule Nürnberg* 26, (April) (2004).
- [16] F. Durst, A new type of internal combustion engine based on the porous-medium combustion in porous medium combustion technique, *Journal of Automobile Engineering* 215 (2) (2001) 63–81.
- [17] M. Jia, M. Xie, A chemical kinetics model of iso-octane oxidation for HCCI engines, *Fuel* 85 (17) (2006) 2593–2604.
- [18] J.B. Heywood, *Internal Combustion Engine Fundamentals*, McGraw-Hill Book Company, New York, 1988. pp. 128–139.
- [19] R.J. Kee, F.M. Rupley, E. Meeks, CHEMKIN-III: a fortran chemical kinetics package for analysis of gas phase chemical and plasma kinetics. Sandia National Laboratory Report CA 94551-0969, 1996.
- [20] J. Chang, O. Güralp, Z. Filipi, D. Assanis, New heat transfer correlation for an HCCI engine derived from measurements of instantaneous surface heat flux. SAE Paper 2004-01-2996, 2004.
- [21] A.J. Barra, J.L. Ellzey, Numerical study of the effects of material properties on flame stabilization in a porous burner, *Combustion and Flame* 134 (3) (2003) 369–379.
- [22] M. Sjöberg, J.E. Dec, Combined effects of fuel-type and engine-speed on intake temperature requirements and completeness of bulk-gas reactions for HCCI combustion, SAE Paper 2003-01-3173, 2003.